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5f. WORK UNIT NUMBER

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14. ABSTRACT
A dedicated high-performance computer cluster was purchased in order to carry out extensive and state-of-the art computations of chemical reaction dynamics. The specific aim of this computational research is the detailed elucidation of the recently reported “roaming” pathway in gas-phase chemical reactions. Several complex reaction systems, currently being studied experimentally will be the focus of this research.

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a. REPORT	b. ABSTRACT	c. THIS PAGE			Joel M Bowman
UU	UU	UU	UU		19b. TELEPHONE NUMBER 404-727-6592

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Report Title

Final Report: High-performance Computer Cluster for Theoretical Studies of Roaming in Chemical Reactions

ABSTRACT

A dedicated high-performance computer cluster was purchased in order to carry out extensive and state-of-the art computations of chemical reaction dynamics. The specific aim of this computational research is the detailed elucidation of the recently reported "roaming" pathway in gas-phase chemical reactions. Several complex reaction systems, currently being studied experimentally will be the focus of this research.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received Paper

TOTAL:

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received Paper

TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Number of Presentations: 0.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received Paper

TOTAL:

Number of Manuscripts:

Books

Received Book

TOTAL:

Received	Book Chapter

TOTAL:

Patents Submitted

Patents Awarded

Awards

Graduate Students

NAME	PERCENT_SUPPORTED

FTE Equivalent:
Total Number:

Names of Post Doctorates

NAME	PERCENT_SUPPORTED

FTE Equivalent:
Total Number:

Names of Faculty Supported

NAME	PERCENT_SUPPORTED

FTE Equivalent:
Total Number:

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED

FTE Equivalent:
Total Number:

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:..... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):..... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:..... 0.00

Names of Personnel receiving masters degrees

NAME

Total Number:

Names of personnel receiving PHDs

NAME

Total Number:

Names of other research staff

NAME	PERCENT_SUPPORTED

FTE Equivalent:

Total Number:

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

A new cluster was purchased from Microway Corporation. Details about this cluster are provided in the attachment to follow

Technology Transfer

Details of the DURIP Cluster Purchase

1. Main purchase, Purchase Order T282738

Oct 16, 2014	T282738	1	Jan 6, 2015

EMORY UNIVERSITY

Atlanta, GA
Emory University is sales tax exempt per Act No. 471 GA Laws 1963.
Fed. Tax exempt no. 58-0566256.
D-U-N-S-06-6469933

Purchasing Contact Information

Contact	Emory University Procurement Operations
Email	e-market@emory.edu
Phone	

Acknowledgements

Advise Procurement Operations if you are unable to fill any part of this order. Email order acknowledgement and shipping date to customer listed below.

Customer Information

Customer Name	Steve Krebs
Customer Email	skrebs@emory.edu

Supplier Information

Supplier Name	MICROWAY INC
Address	12 RICHARDS RD PLYMOUTH, MA 02360 US
Duns No.	
Phone	+1 (508) 325520

Delivery Information

Delivery Address
Emory University

Attn:	Joel Bowman
Department:	Emory University, Chemistry
Building/Room:	109

1515 DICKEY DRIVE
ATLANTA, GA 30322
United States

ShipTo Address Code	EMUNV051

Delivery Information

Requested Delivery Date	
Ship Via	Best Carrier-Best Way

Shipping Instructions

If non-negotiated freight charges apply, ship via FedEx and bill third party to FedEx Account # 342225047 and insert PO# in Recipient 2nd Address field. For free freight and LTL shipments, please use your preferred carrier.

Attachments for supplier

MicroWay MWYQ1604... (185k)

Line No.	Product Description	Catalog No.	Size / Packaging	Unit Price	Quantity	Ext. Price
1 of 4	Microway 2U Xeon Head Node (16 cores @ 2.4GHz; 64GB memory)	unknown	1/EA	6,716.00 USD	1 EA	6,716.00 USD
2 of 4	Microway Xeon 2U Twin² Servers (Four Nodes per 2U)	unknown	1/EA	22,256.00 USD	5 EA	111,280.00 USD
3 of 4	IPMI Management Network	unknown	1/EA	273.00 USD	1 EA	273.00 USD
	Spare Fans	unknown	1/EA	222.00 USD	1 EA	222.00 USD

4 of 4	ATTENTION: IF UNIT COST OF ANY ITEM EXCEEDS THE AMOUNT SHOWN, DO NOT SHIP, CONTACT PROCUREMENT SERVICES AT E-MARKET@EMORY.EDU TO OBTAIN A REVISED PURCHASE ORDER. INVOICES BILLED AT AN AMOUNT HIGHER THAN THAT INDICATED ON THE PURCHASE ORDER WILL BE SHORT-PAID.	Total	**118,491.00 USD**

Billing Information	
Charge to PO Listed Above	
Payment Terms	0% 0, Net 30
F.O.B.	F.O.B Destination
Contract	*no value*
PO Terms	HTTP://TINYURL.COM/EMORYUNIVERSITYPOTERMS

Billing Address
Emory University
Payment Services
PO Box 740046
ATLANTA, GA 30348
United States

PO Terms

Header	Emory University PO Terms	Emory University PO Terms	This Purchase Order is subject to the Purchase Order Terms that are in effect at the time it was distributed to the supplier. Please visit HTTP://TINYURL.COM/EMORYUNIVERSITYPOTERMS to view the complete Emory University Purchase Order Terms.
	Equal Opportunity	Equal Opportunity	The Equal Opportunity Clause, Section 202 of Executive Order 11246, as amended; the Affirmative Action Clause relating to the Rehabilitation Act of 1973, 41CFR 60-250.1, are incorporated herein by reference and shall apply, unless this contract or purchase order is exempted by rules, regulations or orders issued pursuant to Executive Order 11246, the Rehabilitation Act of 1973, the Vietnam Era Veteran's Readjustment Assistance Act of 1972 or provisions of any superseding law or executive order.

2. Expansion to Microway cluster MWYO6655 (PO # T282738) 11/13/15

Total of 4 Compute Nodes:

1	**Microway Xeon 2U Twin² Servers (Four Nodes per 2U)**	$26,507	$19,196	$19,196

NumberSmasher-4X Intel Xeon TwinPro² Servers
2U Rackmount Chassis with
2000W Redundant High-Efficiency Hot-Swap 1+1 Power Supply
26.5" - 36" Rackmount Rail Kit

Four Hot-Pluggable Compute Nodes, each with:

Up to two Intel Xeon E5-2600 Socket R3 processors (up to 120W)
Intel C612 Express chipset
Intel QuickPath Interconnect (QPI) with system bus up to 9.6GT/s
Sixteen slots for up to 1TB ECC DDR4-2133/1866 memory
Dual Integrated Intel i350-AM2 Gigabit Ethernet ports
Integrated LSI 3008 SAS3 (12Gbps) controller
One PCI-Express 3.0 x16 slot (Low Profile; Half-Length)
Integrated ASPEED AST2400 Graphics
IPMI 2.0 w/ Virtual Media, KVM and Dedicated LAN Support
Six hot-swap 2.5" 12Gbps SATA/SAS Drive Bays
Two Stacked USB 3.0 Connectors; One Serial Port; One VGA Port

(8) Intel Xeon E5-2630v3 Haswell-EP 2.40 GHz Eight Core 22nm CPU
with 20MB L3 Cache, DDR4-1866, 8.0 GT/sec QPI, 85W
Supports Hyper-Threading and Turbo Boost up to 3.2 GHz

(2 CPUs per Node)

(32) 16GB DDR4 2133 MHz ECC/Registered Memory (Dual Rank, 1.2V)

(128GB Total Memory per Node @ 1866MHz)

(4) 256GB Samsung 850 Pro Series 2.5" SATA III MLC Solid State Drive
SATA 6Gb/s Interface (Supports 3Gb/s)
Solid State Disk (SSD), 2 Million Hours Mean Time Before Failure (MTBF)
Endurance Rating (Lifetime Writes): 150 TBW, 40GB/day for 10 years
Sustained sequential read: up to 550 MB/s
Sustained sequential write: up to 520 MB/s